

Numerical Simulation of Supersonic Combustion of Hydrogen in a vitiated air stream

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Towards developing predictive models for flows in supersonic combustors, a validation effort to study reactive flows in supersonic combustors was performed using the commercial CFD (Computational Fluid Dynamics) software, FLUENT. A parallel stepped wall injection of hydrogen into a hot vitiated supersonic air stream, for which detailed experimental data was available, was chosen for studying reaction in supersonic flows. The reacting flow study involved the use of a Finite Rate/Eddy dissipation model and a laminar finite-rate chemistry model for turbulence chemistry interaction using different turbulence models. The results for this study compare well with the experimental data, showing that the H₂-Air Global Kinetic mechanism with measured inlet profiles provides a reasonably accurate prediction, with RNG turbulence model using Finite-Rate/eddy dissipation approach for turbulence chemistry interaction..

Keywords: Supersonic flows, chemical kinetics, wall injection, RANS, Turbulence chemistry interaction

Introduction

The development of air breathing hypersonic technologies is of considerable interest all over the world. The scramjet engine is the key enabling technology for sustained hypersonic flight. One of the major technical challenges in a scramjet combustor is the need for having efficient fuel air mixing and combustion in a supersonic stream with the lowest total pressure loss. The task of mixing and combustng supersonically is a daunting one and the simulation of this process can be equally as difficult. A thorough understanding of the phenomena associated with supersonic combustion is necessary for the development and realization of the combustor.

Several configurations for mixing of hydrogen in a supersonic stream have been investigated which have usually involved parallel or angled flow from a stepped wall through a slot configuration and normal or angled flow of hydrogen through arrays of holes of various aspect ratios. Using a parallel stepped wall injection of H₂ into the supersonic combustor is attractive from an experimental study as it involves minimum disturbance of the free stream when fuel and air pressures are matched. Such a study with detailed measurement at the intermediate and exit planes was reported by Burrows and Kurkov which also makes it a good test case for CFD validations.

Many experimental and numerical studies have been conducted in the area of supersonic reacting flows, yet there still remain many issues that are far from being well understood. With the rapid increase and improvement of computational resources it is becoming increasingly feasible to consider many of these issues numerically using computational fluid dynamics (CFD) techniques with improved models and fewer assumptions. While the need for experimentation cannot be downplayed, accurate numerical models can give much needed insight into the physics of reacting supersonic flows. CFD also has the ability to simulate full-size combustors during in-flight conditions, which is easier and much cheaper than full-scale physical testing, especially for large vehicles. However it is necessary that, the numerical algorithms and physical models in use

and in development must be continually validated with experimental data in order to ensure that the predicted results are sufficiently accurate and consistent.

In order to develop better models for describing the supersonic reacting flow field the detailed experimental investigation of Burrows and Kurkov was used for validating and developing the methodology. In the experiment of Burrows and Kurkov, parallel stepped wall injection of Hydrogen into a hot vitiated supersonic stream produced by burning a hydrogen-nitrogen gas mixture with liquid oxygen at high pressure is considered. Detailed measurements of temperature, Mach number and species at the inlet, outlet and an intermediate test section are available to validate the computed results. The simulation was done with different turbulence models and two different turbulence chemistry interaction approaches were employed. The objective of this effort was to assess and identify the better turbulence model among the various RANS models for prediction of such flows.

Computational Model

A two-dimensional domain beginning at the injection step (this was the earliest location where data was available) and ending at the exit of the combustor, as shown in Fig 1 was created and meshed using GAMBIT. To ensure grid independence, the computations were performed with three different grid sizes and a certain grid size which is referred to as the baseline grid, was found to be adequate for the computations and was chosen. The baseline grid which was finally selected after grid independence studies contained 117X69 points and was refined near the wall and injector in the y-direction.

Both pressure based segregated and coupled solvers in FLUENT were used for this case as the coupled solver is recommended for supersonic flow particularly when chemical reactions are being modeled, however for the simulations done in the study no significant improvement with the coupled solver was seen. Five different turbulence models (SKE, RKE, RNG, SST and SA) were used to assess the capability of these models in capturing the flow. The one equation SA model is attractive from the computational economy point of view and is also widely used for modelling supersonic flows. The two equation models like SKE, RKE, RNG and SST models are chosen to assess their ability in capturing the flow structure.

Pressure inlet boundary conditions were used for the vitiated air and H₂ inlets. Profiles for total pressure and total temperature, were specified for the vitiated air inlet using experimental data, whereas constant conditions were set for the H₂ inlet. To assess the importance of the profiles the simulation was also done using constant total pressure and total temperature values for the vitiated air inlet. Walls were set to a constant temperature of 298K, and a pressure outlet condition was used at the exit of the combustor. Rate data for the H₂-O₂ global mechanism available in FLUENT database was used. Viscosity and specific heat were computed using a mass weighted mixing law. The evaluation of specific heat for individual fluids was done by using a temperature dependent piecewise polynomial and for viscosity, Sutherland's law based on temperature was used. The table below shows the test conditions used in the experiment which was simulated computationally. The profiles used for total temperature and total pressure at the inlet of the domain are shown in Fig 2

Inlet conditions used in the experiment

Parameters	Hydrogen Inlet	Vitiated air stream
Mach Number	1.0	2.44
H ₂	1.0	0
H ₂ O	0.0	0.256
O ₂	0.0	0.258
N ₂	0.0	0.486

Both the laminar finite rate kinetics and the finite rate /eddy dissipation model were tried during the course of the validation process using a single-step global reaction mechanism. The laminar kinetics, though strictly valid for

laminar flames, is considered in this case as it is assumed that the effect of turbulent fluctuations can be ignored for supersonic flames as they are negligible. The turbulent fluctuations are considered with the second model with finite rate kinetics. These mechanisms were chosen in order to consider the effect each had on the solution compared to experimental results

Second-order upwind scheme were used for the discretization of convective terms (continuity, momentum, turbulence, energy and species), respectively. Convergence was monitored through the use of residual monitors set to stop the solution once the residuals dropped below a certain value which was chosen as 1×10^{-4} for each parameter. However, for the current reacting flow simulations the residuals typically level off above this value. Convergence was then considered to be achieved once the temperature appeared to stop changing over several hundred iterations. A typical case took approximately 7000 iterations before reaching convergence.

Results and Discussion

The development of the flame structure within the Burrows Kurkov combustor is shown in Fig 3. It is seen that the ignition distance of 18 mm reported in the experimental study is fairly well predicted with the Global kinetic model (21 mm). The plots of total temperature and H_2O mole fraction profiles at the combustor exit predicted by CFD are compared with the experimental data in Fig 4 and 5 considering both uniform profiles for total pressure and total temperature at the vitiated air inlet and with actual measured experimental profiles at the vitiated air inlet. The plots of total temperature and H_2O mass fraction with uniform profiles show a considerable shift near the lower wall. This shift results in over prediction of the measured values along with a shift in the location of the peak temperatures and mole fractions. Using the actual experimental profiles improves the CFD predictions considerably and a closer match with the experimental data is seen. The effect of the different turbulence models in capturing the reacting flow and flame structure with the laminar finite rate kinetics is seen in figs 6-9. These figures show that though the total temperature and the species mass fractions are predicted reasonably well by some of the models like SKE, RNG and SST K- ω , the SA model shows a significant shift towards the bottom wall apparently due to over prediction of mixing between H_2 and air. Similarly the realizable k-e model predicts a highly diffused flame with a very wide reaction zone. The temperature profile with respect to its peak is not matched by any of the models chosen.

The turbulence models which showed a reasonable agreement with data (SKE, RNG and SST K- ω) are further examined using the finite rate/eddy dissipation model in figs 10-13. Thus two turbulence chemistry interaction models are represented in these comparisons: the Global kinetics using laminar chemistry (figs 6-9) and the finite rate/eddy dissipation model where the turbulent fluctuations are considered with the single global reaction. The turbulent chemistry interaction with finite rate/eddy dissipation considerably improves the predictive capability of the models in case of estimation of the total temperature and the species mass fractions. The difference in the temperature and the species fields using the above approach may be explained as follows. Supersonic reacting flows due to the high energies associated with them can give rise to significant temperature and species fluctuations in the reaction zone. The reaction rates are thus strongly affected due to these temperature and concentration changes which are in turn coupled with the turbulent fluctuations. The different way in which this interaction is accounted for while computing the average reaction rates using the laminar finite rate kinetics and the finite rate/eddy dissipation approach in the RANS equations determines the flow field. However the numerical results seem to be shifted and the peak temperature is slightly over-estimated. The apparent shift in these results for the species mass fractions are not caused by a shift of the flame, but are rather a result of reactions taking place over a wider region. A shift in the flame would be noticed by a shift in the temperature curve, which does not take place. Thus it is seen that none of the models could accurately capture both the temperature and species profiles simultaneously. Though the SST model with finite rate /Eddy dissipation captures the peak of the reaction zone well, the temperature values are overestimated. The RNG model is closer to the measured temperature but is slightly shifted. For further clarity fig 14 shows the RNG

model with both laminar finite rate kinetics and the finite rate/eddy dissipation model. The high temperatures in the former case can be attributed to ignoring the dissociation effects due to high static temperatures in the model that are not being considered here as the Global kinetic model is used.

Overall the RNG model with the eddy dissipation/finite rate chemistry appears to be the best when compared with experimental data. It is thought that the limitation in making a better overall prediction is being caused by approximating the reaction with a Global kinetic model instead of an appropriate multistep kinetic mechanism and a lack of using a more rigorous approach for turbulence-chemistry interactions. It was observed that the computational time required with the finite/eddy dissipation was comparable with the laminar finite rate approach. It is also seen that near the lower wall ($y = 0$) the temperature for all the cases is under-estimated, which is apparently due to the use of a constant temperature boundary condition. The walls were not cooled in the experiment, but due to the short run times and good heat sink capacity of the copper wall, it was thought this was a reasonable approximation.

Conclusion

The ability of various turbulence models was assessed in predicting the reacting supersonic turbulent flow with a parallel step wall hydrogen injection into a hot vitiated supersonic air stream. It was seen that among the various turbulence models, the RNG K- ϵ model with the Finite rate/Eddy dissipation scheme provided a relatively better agreement with the experimental results. It was also observed that if measured inlet profiles are used as inputs in the CFD code for vitiated air inlet, the ability of the two equation models in predicting results closer to experimental data is considerably improved even with a Global Kinetic mechanism. The global kinetics also predicts the ignition distances fairly well and is suited for simulations which require quick turnaround times for faster design iterations. However for improving accuracy in capturing the detailed flame structure, detailed kinetics schemes with improved turbulence chemistry interaction models would be needed.

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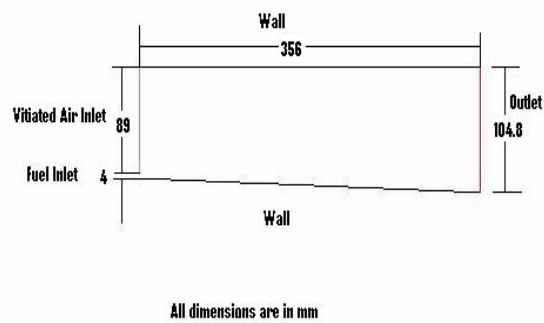


Fig 1: Computational Domain

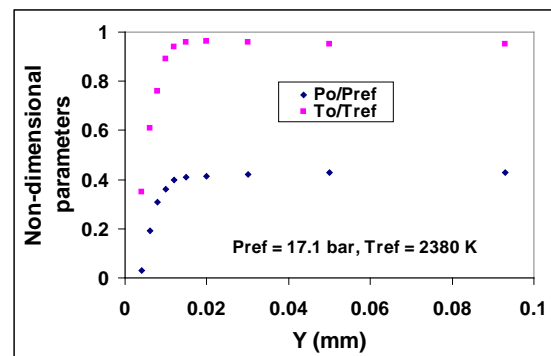


Fig 2: Profiles for Total Pressure and Total Temperature at Vitiated Air Inlet

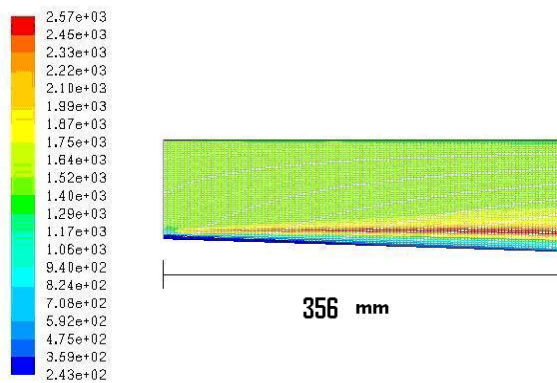
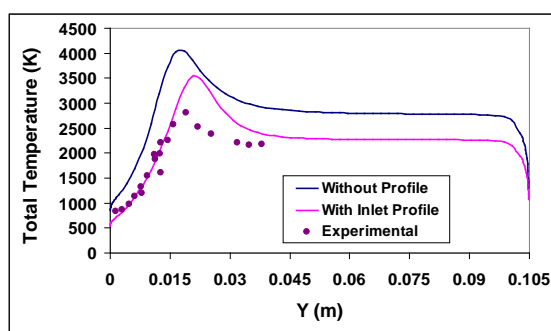
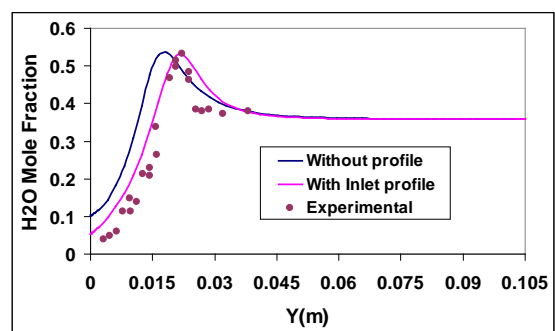
Fig 3: Static temperature contour for SST k- ω turbulence model with Global Finite Rate/Eddy Dissipation.

Fig 4: Total Temperature at Exit with RNG turbulence model, using laminar finite rate model and baseline grid

Fig 5: H₂O Mole Fraction at Exit with RNG turbulence model, using laminar finite rate model and baseline grid

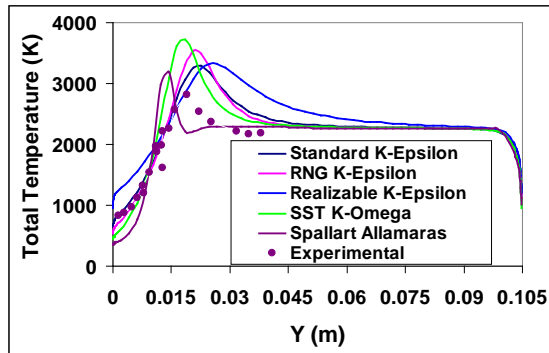


Fig6: Total Temperature at Exit for different turbulence model with Laminar Finite Rate Kinetics, baseline grid

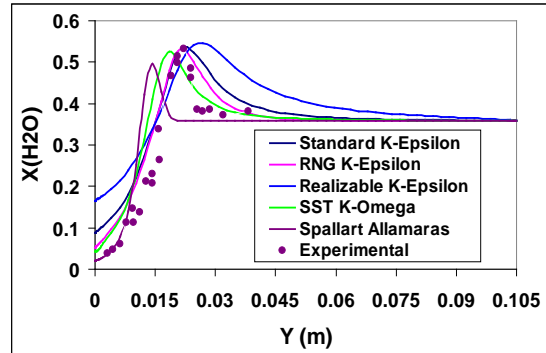


Fig7: H2O Mole Fraction at Exit for different turbulence model with Laminar Finite Kinetics, baseline grid

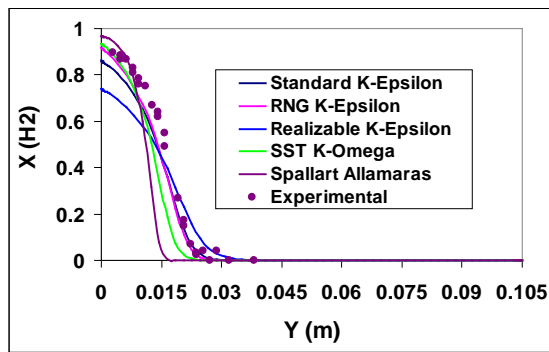


Fig8: H2 Mole Fraction at Exit for different turbulence model with Laminar Finite Rate Kinetics, baseline grid ,

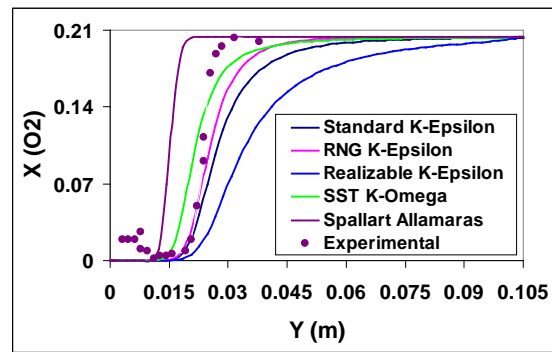


Fig9: O2 Mole Fraction at Exit for different turbulence model with Laminar Finite Rate Kinetics, baseline grid,

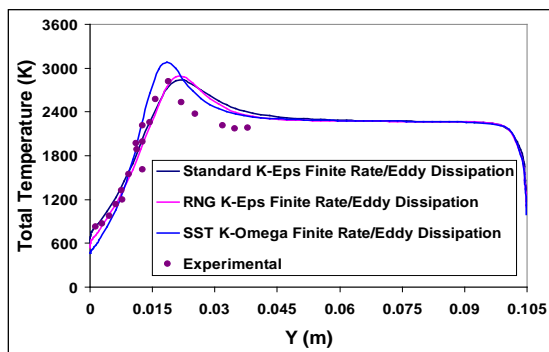


Fig 10: Total Temperature at Exit for different turbulence model with Finite rate/Eddy Dissipation, baseline grid,

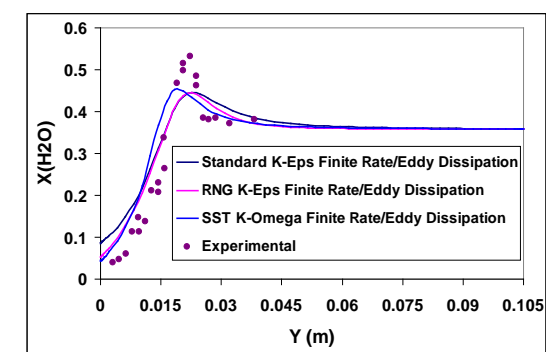


Fig 11: H2O Mole Fraction at Exit for different turbulence model with Finite rate/Eddy Dissipation, baseline grid

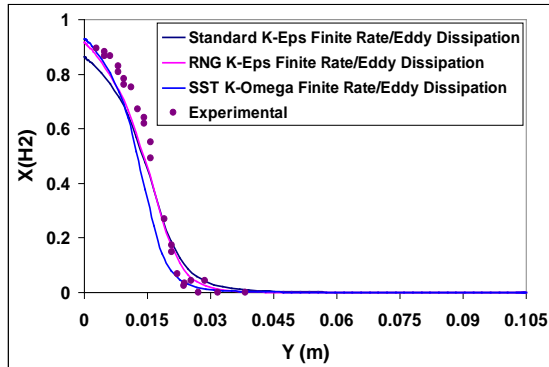


Fig 12: H₂ Mole Fraction at Exit for different turbulence model with Laminar Finite rate kinetics, baseline grid.

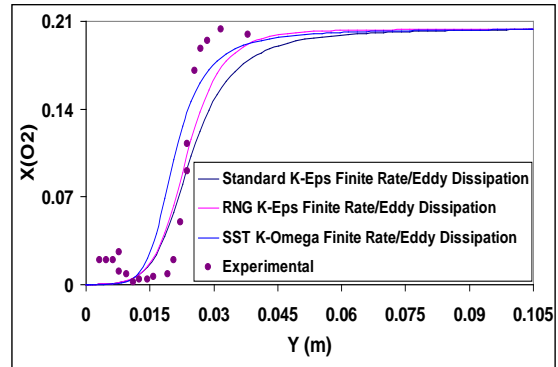


Fig 13: O₂ Mole Fraction at Exit for different turbulence model with Finite rate/Eddy Dissipation, baseline grid.

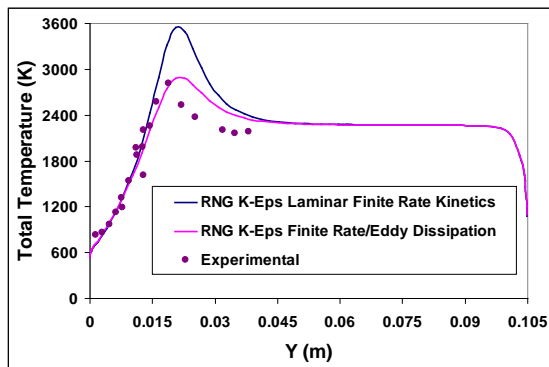


Fig 14: Total Temperature at Exit for different Reaction kinetics with RNG turbulence model, Isothermal wall, baseline grid.